Charged and spin-excitation gaps in half-filled strongly correlated electron systems: A rigorous result

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Abstract

By exploiting the particle-hole symmetries of the Hubbard model, the periodic Anderson model and the Kondo lattice model at half-filling and applying a generalized version of Lieb's spin-reflection positivity method, we show that the charged gaps of these models are always larger than their spin excitation gaps. This theorem confirms the previous results derived by either the variational approach or the density renormalization group approach. 71.27.+a, 71.10.Fd, 75.10.Lp

Since the discovery of high temperature superconductivity in the rare-earthy-based copper oxides[1], interest in the itinerant strongly correlated electron systems has exploded. The main concern of physicists is the interplay between the itinerant magnetism and the metallic behavior in these systems. As the typical models of the strongly correlated electron systems, the Hubbard model[2], the periodic Anderson model[3] and the Kondo lattice model[4] have been widely studied in the past several decades.

To understand the quantum transport and the magnetic properties of the strongly correlated electron systems, many researcher's interests have focused on the charged gaps and the spin excitation gaps in these models at some specific fillings, in particular, at half-filling. For instance, by solving exactly the one-dimensional Hubbard model, Lieb and Wu showed that the model has a nonvanishing charged gap at half-filling for any on-site Coulomb repulsion $U > 0$[5]. Consequently, in one dimension, the half-filled Hubbard model is an insulator. This conclusion is also believed to be true in two dimensions due to the existence of the spin-wave excitations, which is caused by the nesting Fermi surface at half-filling, in the system. On the other hand, the spin excitation gap of the model is closed[6].

For the periodic Anderson model, the situation is more complicated[7],[8],[9],[10]. For instance, by applying the mean field slave-boson theory, Möller and Wölfle showed[8] that there exists a critical value $J_c \equiv 4V^2/U \approx 0.036W$, where W is the bandwidth and equal to $4dt$ for an d-dimensional simple cubic lattice, such that, when the hybridization energy V and the on-site Coulomb repulsion between d-electrons U satisfy $4V^2/U < J_c$, the periodic Anderson model at half-filling has an antiferromagnetic long-range order and the spin excitation gap vanishes. On the other hand, when $4V^2/U > J_c$, the model has a nonvanishing spin excitation gap and its ground state is paramagnetic. The similar conclusions have also been reached by numerical calculations[7]. However, for the Kondo lattice model, such a transition point is absent[11],[12],[13]. By using the density-matrix renormalization group method, Yu and White found that, in one dimension, the spin excitation gap is nonvanishing for any finite exchange interaction $J > 0$ when the model is half-filled[12]. Their result was further confirmed by Shibata *et. al.*[13].

An interesting observation made by these authors is that: *At half-filling, the charged gaps of these models are always larger than their spin excitation gaps*[7],[912]. Therefore, an interesting question arose is whether this observation can be re-established on a more rigorous basis. In this paper, by using a generalized version of Lieb's spin-reflection positivity technique[14],[15],[16],[17], we would like to prove this fact in a mathematically rigorous way. As a by-product of our proof, one can easily see that this observation is a result of the particle-hole symmetry enjoyed by these models at half-filling.

To begin with, we would first like to introduce several definitions and some useful notation.

Take a finite d-dimensional simple cubic lattice Λ with an *even* number of lattice sites and impose the periodic boundary condition on it. Then, the Hamiltonian of the Hubbard model can be written as

$$
\begin{aligned}
H_H = -t \sum_\sigma \sum_{<\mathbf{ij}>} \left(c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{i}\sigma} \right) \\
+ U \sum_{\mathbf{i}\in\Lambda} \left(n_{\mathbf{i}\uparrow} - \frac{1}{2} \right) \left(n_{\mathbf{i}\downarrow} - \frac{1}{2} \right) - \mu \hat{N}
\end{aligned}
\tag{1}
$$

where $c_{\mathbf{i}\sigma}^\dagger$ ($c_{\mathbf{i}\sigma}$) is the fermion creation (annihilation) operator which creates (annihilates) a fermion with spin σ at lattice site $\mathbf{i}$. $n_{\mathbf{i}\sigma} = c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{i}\sigma}$. $< \mathbf{ij} >$ denotes a pair of nearest-neighbor sites of Λ. $t > 0$ and $U > 0$ are two parameters representing the kinetic energy and the screened on-site Coulomb repulsion between fermions, respectively. μ is the chemical potential. With respect to Hamiltonian (1), the simple cubic lattice is bipartite. In other words, it can be split into two separate sublattices A and B such that, the fermion hopping takes place only between sites of different sublattices. In the following, we shall exploit this fact.

Similarly, the Hamiltonians of the symmetric periodic Anderson model and the Kondo lattice model are given by

$$
\begin{aligned}
H_A = -t \sum_\sigma \sum_{<\mathbf{ij}>} \left(c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{i}\sigma} \right) \\
+ V \sum_\sigma \sum_{\mathbf{i}\in\Lambda} \left(c_{\mathbf{i}\sigma}^\dagger d_{\mathbf{i}\sigma} + d_{\mathbf{i}\sigma}^\dagger c_{\mathbf{i}\sigma} \right)
\end{aligned}
$$

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$$+ U \sum_{\mathbf{i} \in \Lambda} \left(d^{\dagger}_{\mathbf{i}\uparrow} d_{\mathbf{i}\uparrow} - \frac{1}{2} \right) \left(d^{\dagger}_{\mathbf{i}\downarrow} d_{\mathbf{i}\downarrow} - \frac{1}{2} \right) - \mu \hat{N} \tag{2}$$

$$H_K = -t \sum_{\sigma} \sum_{\langle \mathbf{ij} \rangle} \left(c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^{\dagger}_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma} \right)$$
$$+ J \sum_{\mathbf{i} \in \Lambda} \sigma_{\mathbf{i}} \cdot \mathbf{s_i} - \mu \hat{N} \tag{3}$$

In Eq. (2), $c_{\mathbf{i}\sigma}$ and $d_{\mathbf{i}\sigma}$ represent the atomic s-orbital and d-orbital fermion operators at lattice site $\mathbf{i}$, respectively. V stands for the hybridization energy of s-electrons and d-electrons. In Eq. (3), $\sigma_{\mathbf{i}}$ and $\mathbf{s_i}$ represent the spin operators of the itinerant electrons and the localized electrons, respectively, and $J > 0$ is the antiferromagnetic exchange interaction between them.

In terms of Hamiltonians (2) and (3), the simple cubic lattice is also bipartite. This fact can be easily understood by introducing a "double layer lattice structure"[18],[19]. For definiteness, let us consider the periodic Anderson model defined on a specific lattice: The two dimensional square lattice with the lattice constant being set to be unit. We take two identical copies of this lattice, Λ_1 and Λ_2, and make a doubly-layered lattice $\widetilde{\Lambda}$ by connecting the corresponding lattice points of Λ_1 and Λ_2 with bonds of length $a = 1$. Now, each point of $\widetilde{\Lambda}$ has coordinates $\mathbf{r} = (\mathbf{i}, m)$ with $m = 1, 2$. Obviously, $\widetilde{\Lambda}$ has $2N_\Lambda$ lattice points. Next, we define new fermion operators $e_{\mathbf{r}\sigma}$ by

$$e_{\mathbf{r}\sigma} = \begin{cases} c_{\mathbf{i}\sigma}, & \text{if } m = 1; \\ d_{\mathbf{i}\sigma}, & \text{if } m = 2. \end{cases} \tag{4}$$

With the definitions of $\widetilde{\Lambda}$ and $e_{\mathbf{r}\sigma}$, the Hamiltonian H_A of the periodic Anderson model can be thought as the Hamiltonian of a generalized Hubbard model on the bipartite lattice $\widetilde{\Lambda}$, if V is taken to be the "hopping energy" of e-electrons between layer 1 and layer 2.

Similarly, for the Kondo lattice, if we re-define the partition of sublattices by the following rule: The hopping energy t and the exchange energy J may be nonzero only for a pair of sites belonging, respectively, to the different sublattices, then lattice $\widetilde{\Lambda}$ as well as the original lattice Λ are apparently bipartite in terms of Hamiltonian (3).

The Hamiltonians H_H, H_A and H_K enjoy several symmetries, which make the analysis of these models easier.

First, Hamiltonians (1), (2) and (3) commute with their total particle number operators $\hat{N}$, respectively. Consequently, their Hilbert spaces can be divided into numerous subspaces $\{V(N)\}$. Each of these subspaces is characterized by an integer N, the total number of fermions in the system. In particular, the subspace $V(N)$ is called the half-filled subspace if $N = N_\Lambda$ for the Hubbard model, $N = 2N_\Lambda$ for both the periodic Anderson model and the Kondo lattice model.

Furthermore, if we define the total spin operators, for the Hubbard model, by

$$\hat{S}_x \equiv \frac{1}{2} \sum_{i\in\Lambda} \left(c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow} \right),$$

$$\hat{S}_y \equiv \frac{1}{2i} \sum_{i\in\Lambda} \left(c_{i\uparrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\uparrow} \right),$$

$$\hat{S}_z \equiv \frac{1}{2} \sum_{i\in\Lambda} \left(n_{i\uparrow} - n_{i\downarrow} \right) \tag{5}$$

for the periodic Anderson model, by

$$\hat{S}_x \equiv \frac{1}{2} \sum_{i\in\Lambda} \left(c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow} + d_{i\uparrow}^\dagger d_{i\downarrow} + d_{i\downarrow}^\dagger d_{i\uparrow} \right),$$

$$\hat{S}_y \equiv \frac{1}{2i} \sum_{i\in\Lambda} \left(c_{i\uparrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\uparrow} + d_{i\uparrow}^\dagger d_{i\downarrow} - d_{i\downarrow}^\dagger d_{i\uparrow} \right),$$

$$\hat{S}_z \equiv \frac{1}{2} \sum_{i\in\Lambda} \left(n_{i\uparrow}^c - n_{i\downarrow}^c + n_{i\uparrow}^d - n_{i\downarrow}^d \right) \tag{6}$$

and, for the Kondo lattice model, by

$$\hat{S}_x \equiv \frac{1}{2} \sum_{i\in\Lambda} \left(c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow} + f_{i\uparrow}^\dagger f_{i\downarrow} + f_{i\downarrow}^\dagger f_{i\uparrow} \right),$$

$$\hat{S}_y \equiv \frac{1}{2i} \sum_{i\in\Lambda} \left(c_{i\uparrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\uparrow} + f_{i\uparrow}^\dagger f_{i\downarrow} - f_{i\downarrow}^\dagger f_{i\uparrow} \right),$$

$$\hat{S}_z \equiv \frac{1}{2} \sum_{i\in\Lambda} \left(n_{i\uparrow}^c - n_{i\downarrow}^c + n_{i\uparrow}^f - n_{i\downarrow}^f \right) \tag{7}$$

then it is easy to check that the Hamiltonians H_H, H_A and H_K commute with their corresponding total spin operators $\hat{S}_+ = \hat{S}_x + i\hat{S}_y$, $\hat{S}_- = \hat{S}_x - i\hat{S}_y$ and $\hat{S}_z$. Consequently, any

eigenstate Ψ_n with quantum number $S^2 = S(S+1)$ of these Hamiltonians must have $2S+1$ isotopes $\{\Psi_n(M)\}$ with $-S \leq M \leq S$.

Here, we would like to emphasize that, in Eq. (7), $f_{\mathbf{i}\sigma}^\dagger$ and $f_{\mathbf{i}\sigma}$ represent the fermion operators of the localized spins. Consequently, they should satisfy the following constraint condition[20]

$$f_{\mathbf{i}\uparrow}^\dagger f_{\mathbf{i}\uparrow} + f_{\mathbf{i}\downarrow}^\dagger f_{\mathbf{i}\downarrow} = 1 \tag{8}$$

This makes them different from operators $c_{\mathbf{i}\sigma}^\dagger$ and $c_{\mathbf{i}\sigma}$, which are the itinerant electron operators.

When the systems are *half-filled*, the chemical potential $\mu = 0$ for all the Hamiltonians H_H, H_A and H_K. This fact is due to the particle-hole symmetry enjoyed by these models at the special filling[21]. As a result, the Hamiltonians H_H, H_A and H_K also commute with the so-called pseudo-spin operators, which are defined, for the Hubbard model[21], by

$$\hat{J}_+ \equiv \sum_{\mathbf{i}\in\Lambda} \epsilon(\mathbf{i}) c_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{i}\downarrow}^\dagger, \quad \hat{J}_- \equiv \hat{J}_+^\dagger,$$
$$\hat{J}_z \equiv \frac{1}{2} \sum_{\mathbf{i}\in\Lambda} (n_{\mathbf{i}\uparrow} + n_{\mathbf{i}\downarrow} - 1) \tag{9}$$

for the symmetric periodic Anderson model[7], by

$$\hat{J}_+ \equiv \sum_{\mathbf{i}\in\Lambda} \epsilon(\mathbf{i}) \left(c_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{i}\downarrow}^\dagger - d_{\mathbf{i}\uparrow}^\dagger d_{\mathbf{i}\downarrow}^\dagger \right), \quad \hat{J}_- \equiv \hat{J}_+^\dagger,$$
$$\hat{J}_z \equiv \frac{1}{2} \sum_{\mathbf{i}\in\Lambda} \left(n_{\mathbf{i}\uparrow}^c + n_{\mathbf{i}\downarrow}^c + n_{\mathbf{i}\uparrow}^d + n_{\mathbf{i}\downarrow}^d - 2 \right) \tag{10}$$

and, for the Kondo lattice model[12], by

$$\hat{J}_+ \equiv \sum_{\mathbf{i}\in\Lambda} \epsilon(\mathbf{i}) \left(c_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{i}\downarrow}^\dagger - f_{\mathbf{i}\uparrow}^\dagger f_{\mathbf{i}\downarrow}^\dagger \right), \quad \hat{J}_- \equiv \hat{J}_+^\dagger,$$
$$\hat{J}_z \equiv \frac{1}{2} \sum_{\mathbf{i}\in\Lambda} \left(n_{\mathbf{i}\uparrow}^c + n_{\mathbf{i}\downarrow}^c + n_{\mathbf{i}\uparrow}^f + n_{\mathbf{i}\downarrow}^f - 2 \right) \tag{11}$$

where $\epsilon(\mathbf{i}) = 1$, for $\mathbf{i} \in A$; $\epsilon(\mathbf{i}) = -1$, for $\mathbf{i} \in B$, is the alternating function. These operators also satisfy the commutation relations of the conventional spin operators. Since H_H, H_A and H_K commute with $\hat{J}_+$, $\hat{J}_-$ and $\hat{J}_z$, both J^2 and J_z are also good quantum numbers and

hence, each eigenstate of H_H, H_A and H_K is characterized by a quantum number J and a quantum number J_z with $-J \leq J_z \leq J$. *It has been shown that, at half-filling, the ground states of the Hubbard model*[15]*, the symmetric periodic Anderson model*[18] *and the Kondo lattice model*[20],[22] *on the simple cubic lattice have quantum numbers $S = 0$ and $J = 0$.*

Next, we would like to introduce the definitions of the charged gaps Δ_c and the spin excitation gaps Δ_s for these strongly-correlated electron models at half-filling. In Refs.[7] and[12], these quantities are defined by

$$\Delta_c \equiv E_0(J = 1,\ S = 0) - E_0(J = 0,\ S = 0),$$
$$\Delta_s \equiv E_0(J = 0,\ S = 1) - E_0(J = 0,\ S = 0) \tag{12}$$

where $E_0(J = j,\ S = s)$ is the lowest eigenvalue of the corresponding Hamiltonian in the subspace with quantum numbers $J = j$ and $S = s$. By using the definitions of the pseudo-spin operators and considering the fact that the ground states of these Hamiltonians at half-filling have quantum numbers $S = 0$ and $J = 0$, the above definitions can be also re-written into the following forms[13], in terms of the total fermion numbers

$$\Delta_c \equiv E_0(\widetilde{N} + 1) + E_0(\widetilde{N} - 1) - 2E_0(\widetilde{N}),$$
$$\Delta_s \equiv E_0(\widetilde{N},\ S = 1) - E_0(\widetilde{N},\ S = 0) \tag{13}$$

where $\widetilde{N} = N_\Lambda$ for the Hubbard model and $\widetilde{N} = 2N_\Lambda$ for both the periodic Anderson model and the Kondo lattice model. Notice that, at half-filling, the Hamiltonians H_H, H_A and H_K enjoy the particle-hole symmetry and hence, identity $E_0(\widetilde{N} + 1) = E_0(\widetilde{N} - 1)$ holds[21]. Therefore, Δ_c can be further written as

$$\Delta_c = 2\left[E_0(\widetilde{N} + 1) - E_0(\widetilde{N})\right] \tag{14}$$

With these preparations, we shall now summarize our main result in the following theorem.

Theorem: For the Hamiltonians H_H, H_A and H_K defined on a d-dimensional simple cubic lattice, when the system is half-filled, the charged gaps and the corresponding spin excitation gaps satisfy the following inequality

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$$\Delta_c \geq \Delta_s \qquad (15)$$

Proof of the theorem: To prove this theorem, we shall apply a generalized version of Lieb's spin-reflection positivity method[15],[16], which we previously used to study the binding energy of fermions in the negative-U Hubbard model[17]. In order to make it more readable, we shall divide the proof of this theorem in several steps:

(1) First, by introducing a unitary partial particle-hole transformation for each model, we map the original Hamiltonians to some equivalent Hamiltonians with *negative* coupling constants.

(2) Then, we write each of the transformed Hamiltonians into a form of the direct product of up-spin fermion operators and down-spin fermion operators.

(3) We shall then apply the spin-reflection positivity method to these transformed Hamiltonians and establish an inequality for the lowest eigenvalues of these transformed Hamiltonians in the different subspaces.

(4) Finally, we apply the inverse of the partial particle-hole transformations to the inequality and finish the proof of the theorem.

In the following, to avoid unnecessary digression, we may directly apply some well-established mathematical results without proving them. Naturally, in that case, we shall refer to some standard references for the reader's convenience.

We now proceed to the proof of the theorem.

Step 1: It is a well-known fact that, for the Hamiltonians H_H, H_A and H_K at half-filling, there exist unitary transformations $\hat{U}_H$, $\hat{U}_A$ and $\hat{U}_K$, which are called the partial particle-hole transformations[21]. Under these transformations, each Hamiltonian with *positive* interaction coupling constants is mapped to a corresponding Hamiltonian with *negative* interactions. To be more precise, let us consider these Hamiltonians one by one.

(a) For the Hubbard Hamiltonian (1), $\hat{U}_H$ is defined by[14],[21]

$$\hat{U}_H^\dagger c_{\mathbf{i}\uparrow} \hat{U}_H = c_{\mathbf{i}\uparrow}, \quad \hat{U}_H^\dagger c_{\mathbf{i}\downarrow} \hat{U}_H = \epsilon(\mathbf{i}) c_{\mathbf{i}\downarrow}^\dagger \qquad (16)$$

At half-filling ($\mu = 0$), under $\hat{U}_H$, H_H is mapped to

$$\widetilde{H}_H = \hat{U}_H^\dagger H_H \hat{U}_H = -t \sum_\sigma \sum_{<\mathbf{ij}>} \left(c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{i}\sigma} \right)$$

$$- U \sum_{\mathbf{i}\in\Lambda} \left(n_{\mathbf{i}\uparrow} - \frac{1}{2} \right) \left(n_{\mathbf{i}\downarrow} - \frac{1}{2} \right) \tag{17}$$

Apparently, $\widetilde{H}_H$ has the same form as H_H. However, in Hamiltonian (17), the sign of U is changed.

(b) For the symmetric periodic Anderson model, the unitary transformation $\hat{U}_A$ is defined by[18]

$$\hat{U}_A^\dagger c_{\mathbf{i}\uparrow} \hat{U}_A = c_{\mathbf{i}\uparrow}, \quad \hat{U}_A^\dagger c_{\mathbf{i}\downarrow} \hat{U}_A = \epsilon(\mathbf{i}) c_{\mathbf{i}\downarrow}^\dagger,$$

$$\hat{U}_A^\dagger f_{\mathbf{i}\uparrow} \hat{U}_A = f_{\mathbf{i}\uparrow}, \quad \hat{U}_A^\dagger f_{\mathbf{i}\downarrow} \hat{U}_A = -\epsilon(\mathbf{i}) f_{\mathbf{i}\downarrow}^\dagger \tag{18}$$

Consequently, under $\hat{U}_A$, H_A is mapped to

$$\widetilde{H}_A = \hat{U}_A^\dagger H_A \hat{U}_A = -t \sum_\sigma \sum_{<\mathbf{ij}>} \left(c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{i}\sigma} \right)$$

$$+ V \sum_\sigma \sum_{\mathbf{i}\in\Lambda} \left(c_{\mathbf{i}\sigma}^\dagger d_{\mathbf{i}\sigma} + d_{\mathbf{i}\sigma}^\dagger c_{\mathbf{i}\sigma} \right)$$

$$- U \sum_{\mathbf{i}\in\Lambda} \left(n_{\mathbf{i}\uparrow}^d - \frac{1}{2} \right) \left(n_{\mathbf{i}\downarrow}^d - \frac{1}{2} \right) \tag{19}$$

Notice that the sign of U is changed but the sign of V is invariant. Since the hybridization term can be mathematically treated as a generalized "hopping" term, as we shall show, the sign of V plays no role in the following proof.

(c) For the Kondo lattice model, the unitary partial particle-hole transformation $\hat{U}_K$ is given by[20]

$$\hat{U}_K^\dagger c_{\mathbf{i}\uparrow} \hat{U}_K = c_{\mathbf{i}\uparrow}, \quad \hat{U}_K^\dagger c_{\mathbf{i}\downarrow} \hat{U}_K = \epsilon(\mathbf{i}) c_{\mathbf{i}\downarrow}^\dagger,$$

$$\hat{U}_K^\dagger f_{\mathbf{i}\uparrow} \hat{U}_K = f_{\mathbf{i}\uparrow}, \quad \hat{U}_K^\dagger f_{\mathbf{i}\downarrow} \hat{U}_K = -\epsilon(\mathbf{i}) f_{\mathbf{i}\downarrow}^\dagger \tag{20}$$

Under $\hat{U}_K$, the constraint condition (8) now reads

$$f_{\mathbf{i}\uparrow}^\dagger f_{\mathbf{i}\uparrow} = f_{\mathbf{i}\downarrow}^\dagger f_{\mathbf{i}\downarrow} \tag{21}$$

and the half-filled Hamiltonian H_K is mapped to[22]

$$\widetilde{H}_K = \hat{U}_K^\dagger H_K \hat{U}_K = -t \sum_\sigma \sum_{\langle \mathbf{ij} \rangle} \left(c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + c_{\mathbf{j}\sigma}^\dagger c_{\mathbf{i}\sigma} \right)$$

$$- \frac{J}{4} \sum_\sigma \sum_{\mathbf{i} \in \Lambda} \left(c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{i}\sigma} + f_{\mathbf{i}\sigma}^\dagger f_{\mathbf{i}\sigma} \right)$$

$$+ \frac{J}{2} \sum_{\mathbf{i} \in \Lambda} \left(c_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{i}\uparrow} f_{\mathbf{i}\uparrow}^\dagger f_{\mathbf{i}\uparrow} + c_{\mathbf{i}\downarrow}^\dagger c_{\mathbf{i}\downarrow} f_{\mathbf{i}\downarrow}^\dagger f_{\mathbf{i}\downarrow} \right)$$

$$- \frac{J}{2} \sum_{\mathbf{i} \in \Lambda} \left(c_{\mathbf{i}\uparrow}^\dagger f_{\mathbf{i}\uparrow} c_{\mathbf{i}\downarrow}^\dagger f_{\mathbf{i}\downarrow} + f_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{i}\uparrow} f_{\mathbf{j}\downarrow}^\dagger c_{\mathbf{i}\downarrow} \right) \qquad (22)$$

We notice that, in Hamiltonian (22), the sign of the last term is *negative*. This fact is the basis of our proof of the theorem for the Kondo lattice model. The first three terms can be mathematically treated as generalized "hopping" terms. We shall see that their signs do not matter.

Here, we would like to make some remarks.

Remark 1: Under $\hat{U}_H$, $\hat{U}_A$ and $\hat{U}_K$, *the half-filled subspace for the corresponding Hamiltonian is mapped into itself.* In particular, since these transformations are unitary, the ground states of H_H, H_A and H_K in the half-filled subspace $V(\widetilde{N})$ are mapped onto their counterparts for $\widetilde{H}_H$, $\widetilde{H}_A$ and $\widetilde{H}_K$ in the same subspace. However, other subspaces are not invariant under these transformations.

Remark 2: Under the partial particle-hole transformations, the spin operators $\hat{S}_+$, $\hat{S}_-$ and $\hat{S}_z$ related to each Hamiltonian are mapped onto the corresponding pseudo-spin operators $\hat{J}_+$, $\hat{J}_-$ and $\hat{J}_z$, and vice versa. Consequently, under these transformations, an eigenstate $\Psi(J = j, S = s)$ of the original Hamiltonians $H_{H,\,A,\,K}$ is mapped onto an eigenstate $\widetilde{\Psi}(J = s,\, S = j)$ of the transformed Hamiltonians $\widetilde{H}_{H,\,A,\,K}$. In particular, the ground states of the original Hamiltonians in the sector with quantum numbers $J = j$, $S = s$ is mapped to the ground states of the transformed Hamiltonians in the sector with quantum numbers $J = s$, $S = j$. This observation is important in carrying out our proof in Step 4.

Step 2. Next, we would like to write Hamiltonians (17), (19) and (22) into a form of the direct product of up-spin fermion operators with down-spin fermion operators. For this purpose, we shall follow Ref.[16] and introduce the following new fermion operators for each Hamiltonian. We let

$$\hat{C}_{\mathbf{i}\uparrow} \equiv e_{\mathbf{i}\uparrow}, \quad \hat{C}_{\mathbf{i}\downarrow} \equiv (-1)^{\hat{N}_\uparrow} e_{\mathbf{i}\downarrow} \tag{23}$$

where $e_{\mathbf{i}\sigma}$ stands for $c_{\mathbf{i}\sigma}$, $f_{\mathbf{i}\sigma}$ and $d_{\mathbf{i}\sigma}$ appearing in Eqs. (17), (19) and (22), respectively. $N_\uparrow$ is the total number of fermions with up-spin in the system. Here, we would like to emphasize that the new fermion operators $\{\hat{C}_{\mathbf{i}\downarrow}\}$, now, *commute with* $\{\hat{C}_{\mathbf{i}\uparrow}\}$. Consequently, Hamiltonians (17), (19) and (22) can be, respectively, re-written as

$$
\begin{aligned}
\widetilde{H}_H = {}& \hat{T}_\uparrow \otimes \hat{I} + \hat{I} \otimes \hat{T}_\downarrow \\
& - U \sum_{\mathbf{i}\in\Lambda} \left(\hat{n}_{\mathbf{i}\uparrow} - \frac{1}{2} \right) \otimes \left(\hat{n}_{\mathbf{i}\downarrow} - \frac{1}{2} \right)
\end{aligned}
\tag{24}
$$

$$
\begin{aligned}
\widetilde{H}_A = {}& \hat{T}'_\uparrow \otimes \hat{I} + \hat{I} \otimes \hat{T}'_\downarrow \\
& - U \sum_{\mathbf{i}\in\Lambda} \left(\hat{n}^d_{\mathbf{i}\uparrow} - \frac{1}{2} \right) \otimes \left(\hat{n}^d_{\mathbf{i}\downarrow} - \frac{1}{2} \right)
\end{aligned}
\tag{25}
$$

and

$$
\begin{aligned}
\widetilde{H}_K = {}& \hat{T}''_\uparrow \otimes \hat{I} + \hat{I} \otimes \hat{T}''_\downarrow \\
& - \frac{J}{2} \sum_{\mathbf{i}\in\Lambda} \left(c^\dagger_{\mathbf{i}\uparrow} f_{\mathbf{i}\uparrow} \otimes c^\dagger_{\mathbf{i}\downarrow} f_{\mathbf{i}\downarrow} + f^\dagger_{\mathbf{i}\uparrow} c_{\mathbf{i}\uparrow} \otimes f^\dagger_{\mathbf{j}\downarrow} c_{\mathbf{i}\downarrow} \right)
\end{aligned}
\tag{26}
$$

In Eqs. (24), (25) and (26), $\hat{T}_\sigma$, $\hat{T}'_\sigma$ and $\hat{T}''_\sigma$ are some Hermitian polynomials of the fermion operators of spin σ. $\hat{I}$ is the identity operator. Apparently, all the above Hamiltonians can be written in the following standard form

$$
\begin{aligned}
\widetilde{H} = {}& \hat{G}_\uparrow \otimes \hat{I} + \hat{I} \otimes \hat{G}_\downarrow \\
& - \lambda \sum_{\mathbf{i}\in\Lambda} \left(\hat{Q}_{\mathbf{i}\uparrow} \otimes \hat{Q}_{\mathbf{i}\downarrow} + \hat{Q}^\dagger_{\mathbf{i}\uparrow} \otimes \hat{Q}^\dagger_{\mathbf{i}\downarrow} \right)
\end{aligned}
\tag{27}
$$

where λ is a *positive* constant. We notice that all the operators $\{\hat{Q}_{\mathbf{i}\sigma}\}$ and $\{\hat{Q}^\dagger_{\mathbf{i}\sigma}\}$ in Eq. (27) are *real operators*. In other words, they are polynomials of $\hat{C}_{\mathbf{i}\sigma}$ and $\hat{C}^\dagger_{\mathbf{i}\sigma}$ with *real coefficients*. The fact is of fundamental importance for applying Lieb's spin-reflection positivity method. Now, we are able to treat $\widetilde{H}_H$, $\widetilde{H}_A$ and $\widetilde{H}_K$ simultaneously, by studying the standard Hamiltonian (27).

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Step 3: Now, let us consider the ground state $\Psi_0(\widetilde{N}+1)$ of $\widetilde{H}$ in the subspace $V(\widetilde{N}+1)$. Since the spin operators $\hat{S}_+$ and $\hat{S}_-$ commute with $\widetilde{H}$, by applying these operators an appropriate number of times, we can always transform $\Psi_0(\widetilde{N}+1)$ into a state satisfying the condition $N_\uparrow - N_\downarrow = 1$. This state has quantum number $S_z = \frac{1}{2}$. In the following, we shall exclusively use $\Psi_0(\widetilde{N}+1)$ to denote this state.

The wave function $\Psi_0(\widetilde{N}+1)$, which has $\frac{\widetilde{N}}{2}+1$ up-spin fermions and $\frac{\widetilde{N}}{2}$ down-spin fermions, can be written as

$$\Psi_0(\widetilde{N}+1) = \sum_{m,\,n} W_{mn} \chi_m^\uparrow \otimes \chi_n^\downarrow \tag{28}$$

In Eq. (28), χ_k^σ is a state vector defined by

$$\chi_k^\sigma \equiv \hat{C}_{\mathbf{i}_1\sigma}^\dagger \cdots \hat{C}_{\mathbf{i}_M\sigma}^\dagger \,|\,0\rangle \tag{29}$$

where $(\mathbf{i}_1,\ldots,\mathbf{i}_M)$, $M = \frac{\widetilde{N}}{2}+1$, for $\sigma =\uparrow$; $M = \frac{\widetilde{N}}{2}$, for $\sigma =\downarrow$, denote the positions of fermions with spin σ. We would like to emphasize that, when $\widetilde{H} = \widetilde{H}_K$, the constraint condition (21) should be taken into consideration to determine the coefficients $\{W_{mn}\}$ of the ground state wave function. Apparently, the entire set $\{\chi_k^\sigma\}$ gives a natural basis for $V_\sigma(M)$, the subspace of M fermions with spin σ. However, we should notice that, if we naively choose $\mathcal{H}_\uparrow = V_\uparrow(\frac{\widetilde{N}}{2}+1)$ and $\mathcal{H}_\downarrow = V_\downarrow(\frac{\widetilde{N}}{2})$ to be the subspaces for up-spin and down-spin fermions, then the coefficient matrix $\mathcal{W} = (W_{mn})$ will be an $C_{\widetilde{N}}^{\widetilde{N}/2+1} \times C_{\widetilde{N}}^{\widetilde{N}/2}$ matrix, *which is not a square matrix*. Mathematically, it is rather difficult to deal with such a matrix. To avoid this nuisance, we shall define both $\mathcal{H}_\uparrow$ and $\mathcal{H}_\downarrow$ by $\mathcal{H}_\sigma = V_\sigma(\frac{\widetilde{N}}{2}) \oplus V_\sigma(\frac{\widetilde{N}}{2}+1)$. Consequently, $\mathcal{H}_\uparrow$ and $\mathcal{H}_\downarrow$ have the same dimension and hence, matrix $\mathcal{W}$ can now be written as an $D \times D$ *square matrix* with $D = C_{\widetilde{N}}^{\widetilde{N}/2} + C_{\widetilde{N}}^{\widetilde{N}/2+1}$. Explicitly, we have

$$\mathcal{W} = \begin{pmatrix} O & \mathcal{M} \\ O & O \end{pmatrix} \tag{30}$$

In Eq. (30), $\mathcal{M}$ is an $C_{\widetilde{N}}^{\widetilde{N}/2+1} \times C_{\widetilde{N}}^{\widetilde{N}/2}$ nonzero matrix and O represents zero matrices. In terms of matrix $\mathcal{W}$, the normalization of $\Psi_0(\widetilde{N}+1)$ is now given by $\mathrm{Tr}\mathcal{W}^\dagger\mathcal{W} = 1$.

For such a square matrix, we have the following polar factorization lemma in matrix theory.

Lemma: Let A be an *arbitrary* (Not necessarily Hermitian) $n \times n$ matrix. Then, there are two $n \times n$ *unitary* matrices U, V and an $n \times n$ *diagonal* semi-positive definite matrix H such that

$$A = UHV,$$

$$h_{mn} = h_m \delta_{mn} \text{ and } h_m \geq 0, \quad m = 1, \cdots, n. \tag{31}$$

One can find the proof of this lemma in a standard textbook of matrix theory[23] or read the appendix of Ref.[17].

Applying this lemma, we can find two unitary matrices U, V and a diagonal positive semidefinite matrix H, such that $\mathcal{W} = UHV$. Consequently, $\Psi_0(\widetilde{N} + 1)$ can be re-written as

$$
\begin{aligned}
\Psi_0(\widetilde{N} + 1) &= \sum_{m=1}^{D} \sum_{n=1}^{D} W_{mn} \chi_m^{\uparrow} \otimes \chi_n^{\downarrow} \\
&= \sum_{m=1}^{D} \sum_{n=1}^{D} (UHV)_{mn} \chi_m^{\uparrow} \otimes \chi_n^{\downarrow} \\
&= \sum_{l=1}^{D} h_l \psi_l^{\uparrow} \otimes \phi_l^{\downarrow}
\end{aligned}
\tag{32}
$$

with

$$\psi_l^{\uparrow} = \sum_{m=1}^{D} U_{ml} \chi_m^{\uparrow}, \quad \phi_l^{\downarrow} = \sum_{n=1}^{D} V_{ln} \chi_n^{\downarrow} \tag{33}$$

Since U and V are unitary, $\{\psi_l^{\uparrow}\}$ and $\{\phi_l^{\downarrow}\}$ are also orthonormal bases in subspaces $\mathcal{H}_{\uparrow}$ and $\mathcal{H}_{\downarrow}$, respectively. Furthermore, since $\Psi_0(\widetilde{N} + 1)$ is an eigenvector of $\hat{N}_{\uparrow}$, we have

$$\hat{N}_{\uparrow} \mid \Psi_0(\widetilde{N} + 1)\rangle = \left(\frac{\widetilde{N}}{2} + 1 \right) \mid \Psi_0(\widetilde{N} + 1)\rangle \tag{34}$$

or, equivalently,

$$
\begin{aligned}
\sum_{l=1}^{D} h_l \left[\hat{N}_{\uparrow} \psi_l^{\uparrow} \right] \otimes \phi_l^{\downarrow} \\
= \sum_{l=1}^{D} h_l \left[\left(\frac{\widetilde{N}}{2} + 1 \right) \psi_l^{\uparrow} \right] \otimes \phi_l^{\downarrow}
\end{aligned}
\tag{35}
$$

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Taking the inner product of Eq. (35) with $\phi_{l'}^{\downarrow}$ projects out

$$h_{l'}\left[\hat{N}_{\uparrow}\psi_{l'}^{\uparrow}\right] = h_{l'}\left[\left(\frac{\widetilde{N}}{2}+1\right)\psi_{l'}^{\uparrow}\right] \tag{36}$$

Consequently, the corresponding state $\psi_l^{\uparrow}$ is an *eigenvector* of $\hat{N}_{\uparrow}$ with eigenvalue $\widetilde{N}/2 + 1$, if $h_l \neq 0$. The same conclusion can also be reached for operator $\hat{N}_{\downarrow}$ and states $\{\phi_l^{\downarrow}\}$.

For technical reasons, the above conclusions are generally written in the following weaker form

$$\langle \Psi_0(\widetilde{N}+1) \mid \hat{N}_{\uparrow} \mid \Psi_0(\widetilde{N}+1)\rangle$$
$$= \sum_{l=1}^{D} h_l^2 \langle \psi_l \mid \hat{N} \mid \psi_l\rangle = \frac{\widetilde{N}}{2} + 1 \tag{37}$$

and

$$\langle \Psi_0(\widetilde{N}+1) \mid \hat{N}_{\downarrow} \mid \Psi_0(\widetilde{N}+1)\rangle$$
$$= \sum_{l=1}^{D} h_l^2 \langle \phi_l \mid \hat{N} \mid \phi_l\rangle = \frac{\widetilde{N}}{2} \tag{38}$$

In both Eqs. (37) and (38), the spin indices are dropped in the sums, because, in each equation, only one species of spin is involved. These equations are particularly useful in proving the strictness of inequality (15) for a *finite* system (See Ref.[17] for details) and will be used in the following.

In terms of Eq. (32), the ground state energy of $\widetilde{H}$ in subspace $V(\widetilde{N}+1)$ is now given by

$$E_0(\widetilde{N}+1)$$
$$= \langle \Psi_0(\widetilde{N}+1) \mid \widetilde{H} \mid \Psi_0(\widetilde{N}+1)\rangle$$
$$= \sum_{l=1}^{D} h_l^2 \left[\langle \psi_l^{\uparrow} \mid \hat{G}_{\uparrow} \mid \psi_l^{\uparrow}\rangle + \langle \phi_l^{\downarrow} \mid \hat{G}_{\downarrow} \mid \phi_l^{\downarrow}\rangle\right]$$
$$- \lambda \sum_{\mathbf{i}\in\Lambda} \left(\sum_{l_1,l_2=1}^{D} h_{l_1} h_{l_2} \langle \psi_{l_2}^{\uparrow} \mid \hat{Q}_{\mathbf{i}\uparrow} \mid \psi_{l_1}^{\uparrow}\rangle\langle \phi_{l_2}^{\downarrow} \mid \hat{Q}_{\mathbf{i}\downarrow} \mid \phi_{l_1}^{\downarrow}\rangle\right)$$
$$- \lambda \sum_{\mathbf{i}\in\Lambda} \left(\sum_{l_1,l_2=1}^{D} h_{l_1} h_{l_2} \langle \psi_{l_2}^{\uparrow} \mid \hat{Q}_{\mathbf{i}\uparrow}^{\dagger} \mid \psi_{l_1}^{\uparrow}\rangle\langle \phi_{l_2}^{\downarrow} \mid \hat{Q}_{\mathbf{i}\downarrow}^{\dagger} \mid \phi_{l_1}^{\downarrow}\rangle\right) \tag{39}$$

Applying inequality $\mid ab \mid \leq \frac{1}{2}(\mid a \mid^2 + \mid b \mid^2)$ to each term in the triple summations and dropping the spin indices, we obtain

$$
\begin{aligned}
E_0(\widetilde{N} + 1) \\
\geq \frac{1}{2} \sum_{l=1}^{D} h_l^2 \left[\langle \psi_l \mid \hat{G} \mid \psi_l \rangle + \langle \psi_l \mid \hat{G} \mid \psi_l \rangle \right] \\
+ \frac{1}{2} \sum_{l=1}^{D} h_l^2 \left[\langle \phi_l \mid \hat{G} \mid \phi_l \rangle + \langle \phi_l \mid \hat{G} \mid \phi_l \rangle \right] \\
- \frac{\lambda}{2} \sum_{\mathbf{i} \in \Lambda} \left(\sum_{l_1, l_2 = 1}^{D} h_{l_1} h_{l_2} \langle \psi_{l_2} \mid \hat{Q}_{\mathbf{i}} \mid \psi_{l_1} \rangle \overline{\langle \psi_{l_2} \mid \hat{Q}_{\mathbf{i}} \mid \psi_{l_1} \rangle} \right) \\
- \frac{\lambda}{2} \sum_{\mathbf{i} \in \Lambda} \left(\sum_{l_1, l_2 = 1}^{D} h_{l_1} h_{l_2} \langle \phi_{l_2} \mid \hat{Q}_{\mathbf{i}} \mid \phi_{l_1} \rangle \overline{\langle \phi_{l_2} \mid \hat{Q}_{\mathbf{i}} \mid \phi_{l_1} \rangle} \right) \\
- \frac{\lambda}{2} \sum_{\mathbf{i} \in \Lambda} \left(\sum_{l_1, l_2 = 1}^{D} h_{l_1} h_{l_2} \langle \psi_{l_2} \mid \hat{Q}_{\mathbf{i}}^\dagger \mid \psi_{l_1} \rangle \overline{\langle \psi_{l_2} \mid \hat{Q}_{\mathbf{i}}^\dagger \mid \psi_{l_1} \rangle} \right) \\
- \frac{\lambda}{2} \sum_{\mathbf{i} \in \Lambda} \left(\sum_{l_1, l_2 = 1}^{D} h_{l_1} h_{l_2} \langle \phi_{l_2} \mid \hat{Q}_{\mathbf{i}}^\dagger \mid \phi_{l_1} \rangle \overline{\langle \phi_{l_2} \mid \hat{Q}_{\mathbf{i}}^\dagger \mid \phi_{l_1} \rangle} \right) \quad (40)
\end{aligned}
$$

Next, we introduce new wave functions Ψ_1 and Ψ_2 by

$$
\Psi_1 = \sum_{l=1}^{D} h_l \psi_l^\uparrow \otimes \bar{\psi}_l^\downarrow, \quad \Psi_2 = \sum_{l=1}^{D} h_l \phi_l^\uparrow \otimes \bar{\phi}_l^\downarrow \quad (41)
$$

where $\bar{\psi}_l$ and $\bar{\phi}_l$ are the complex conjugates of ψ_l and ϕ_l, respectively. Apparently, we have

$$
\begin{aligned}
\langle \Psi_1 \mid \Psi_1 \rangle = \langle \Psi_2 \mid \Psi_2 \rangle \\
= \sum_{l=1}^{D} h_l^2 = \langle \Psi_0(\widetilde{N} + 1) \mid \Psi_0(\widetilde{N} + 1) \rangle = 1 \quad (42)
\end{aligned}
$$

Since $\hat{G}$ is hermitian and $\{\hat{Q}_{\mathbf{i}}\}$ ($\{\hat{Q}_{\mathbf{i}}^\dagger\}$) are *real*, in terms of Ψ_1 and Ψ_2, inequality (40) can be re-written as

$$
E_0(\widetilde{N} + 1) \geq \frac{1}{2} \langle \Psi_1 \mid \widetilde{H} \mid \Psi_1 \rangle + \frac{1}{2} \langle \Psi_2 \mid \widetilde{H} \mid \Psi_2 \rangle \quad (43)
$$

On the other hand, we notice that Ψ_1 and Ψ_2 are actually wave functions in subspace $V(\frac{\widetilde{N}}{2} + 1, \frac{\widetilde{N}}{2} + 1)$ and $V(\frac{\widetilde{N}}{2}, \frac{\widetilde{N}}{2})$, respectively. For example, by using the constraint condition (37), we have

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$$\langle \Psi_1 \mid \hat{N}_\uparrow \mid \Psi_1 \rangle = \langle \Psi_1 \mid \hat{N}_\downarrow \mid \Psi_1 \rangle$$

$$= \sum_{l=1}^{D} h_l^2 \langle \psi_l \mid \hat{N} \mid \psi_l \rangle = \frac{\widetilde{N}}{2} + 1 \qquad (44)$$

Therefore, by the variational principle, we obtain

$$E_0(\widetilde{N}+1) \geq \frac{1}{2} E_0(\widetilde{N}+2) + \frac{1}{2} E_0(\widetilde{N}) \qquad (45)$$

Remark 3: We should notice that, while the construction of Ψ_1 and Ψ_2 for both $\widetilde{H}_H$ and $\widetilde{H}_A$ is straightforward, the job should be done in a more cautious way as far as $\widetilde{H}_K$ is concerned. We should show that both Ψ_1 and Ψ_2 satisfy the constraint condition (21). That can be achieved in the following way.

By reorganizing the rows and columns of the coefficient matrix $\mathcal{W}$ (by a unitary transformation), we can always write it in a "block diagonal" form: $\mathcal{W} = diag\,(\mathcal{W}_1, \mathcal{W}_2, \cdots)$, where each block $\mathcal{W}_k$ is a *square matrix* and corresponds to a sector in which the distribution of f-fermions is specified, subject to the condition (21). Naturally, $\mathcal{W}_k$ has also the form of Eq. (30). Applying the lemma to each of these submatrices $\{\mathcal{W}_k\}$, we can construct unitary matrices U and V with the following block diagonal form:

$$U = diag\,(U_1, U_2, \cdots), \quad V = diag\,(V_1, V_2, \cdots) \qquad (46)$$

and diagonalize the coefficient matrix $\mathcal{W}$ by them. Now, it is easy to see that the wave functions Ψ_1 and Ψ_2 constructed according to the above-mentioned rule satisfy the constraint condition (21).

Step 4: Finally, we apply the inverse of $\hat{U}_H$, $\hat{U}_A$ and $\hat{U}_K$ to map the "negative coupling" Hamiltonians $\widetilde{H}_H$, $\widetilde{H}_A$ and $\widetilde{H}_K$ back onto the original Hamiltonians H_H, H_A and H_K. We are mainly interested in the change of inequality (45) under these transformations. For this purpose, let us consider how each of $E_0(\widetilde{N})$, $E_0(\widetilde{N}+1)$ and $E_0(\widetilde{N}+2)$ changes under the unitary inverse transformations.

First, as we mentioned in Remark 2, $E_0(\widetilde{N})$ is *unchanged* under the partial particle-hole transformations. In other words, it still presents the lowest eigenvalues of the original

Hamiltonians H_H, H_A and H_K in the half-filled subspace $V(N = \widetilde{N})$. Interestingly, $E_0(\widetilde{N}+1)$ is also invariant. This is due to the fact that the partial particle-hole transformations only change the particle number of down-spin fermions from $\frac{\widetilde{N}}{2}$ to $\widetilde{N} - \frac{\widetilde{N}}{2} = \frac{\widetilde{N}}{2}$ and keep the particle number of up-spin fermions, $N_\uparrow = \frac{\widetilde{N}}{2} + 1$ unchanged. Consequently, the subspace $V(N_\uparrow = \frac{\widetilde{N}}{2} + 1, \ N_\downarrow = \frac{\widetilde{N}}{2})$ is unitarily mapped into itself. However, the change of $E_0(\widetilde{N} + 2)$ demands a careful consideration.

It has been previously proven that, in the subspace $V(\widetilde{N} + 2)$, the ground states of the Hamiltonians $\widetilde{H}_H$[14],[15], $\widetilde{H}_A$[18] and $\widetilde{H}_K$[20],[22] have quantum numbers $S = 0$ and $J = 1$. Therefore, under the inverse transformations $\hat{U}_H^{-1}$, $\hat{U}_A^{-1}$ and $\hat{U}_K^{-1}$, these states are mapped onto the ground states of the *original Hamiltonians H_H, H_A and H_K* in the subspace with quantum numbers $J = 0$ and $S = 1$, as we discussed above in Remark 2. In other words, these states are the ground states of the original Hamiltonians in the half-filled sector with $S = 1$. Consequently, we obtain

$$E_0(\widetilde{N} + 2; \ \widetilde{H}_{H,A,K}) = E_0(\widetilde{N}, \ S = 1; \ H_{H,A,K}) \tag{47}$$

Therefore, for the Hamiltonians H_H, H_A and H_K, inequality (45) now reads

$$E_0(\widetilde{N} + 1) \geq \frac{1}{2} E_0(\widetilde{N}, \ S = 1) + \frac{1}{2} E_0(\widetilde{N}, \ S = 0) \tag{48}$$

or, equivalently

$$\begin{aligned} &E_0(\widetilde{N} + 1) - E_0(\widetilde{N}) \\ &\geq \frac{1}{2} E_0(\widetilde{N}, \ S = 1) - \frac{1}{2} E_0(\widetilde{N}, \ S = 0) \end{aligned} \tag{49}$$

Multiplying both sides of inequality (49) by 2, we obtain inequality (15). That ends our proof of the theorem. **QED**.

Some remarks are in order.

Remark 4: Actually, inequality (49) can be slightly strengthened for the Hubbard model and the symmetric periodic Anderson model at half-filling. Following Ref.[17], one can easily show that, for any *finite* lattice Λ, inequality (49) is *strict*. In other words, the systems have

a Mott charged gap. However, in the thermodynamic limit, the inequality resumes the form of Eq. (49). Therefore, to study the Mott metal-insulator transition of these models in the thermodynamic limit, one needs to introduce some more sophisticated method.

Remark 5: In the above proof, we assumed that the coupling constants in each Hamiltonian are site-independent. That is only a harmless assumption to make our proof simpler. Actually, inequalities (45) as well as (49) still hold for the models with *site-dependent* coupling constants and its proof is essentially unchanged. One can find more details in Ref.[17].

In summary, in this article, by exploiting the partial particle-hole symmetry of the Hubbard model, the periodic Anderson model and the Kondo lattice model at half-filling and applying a generalized version of Lieb's spin-reflection positivity method, we proved that the charged gaps of these models are always larger than their spin excitation gaps. This theorem confirms the previous results derived by either the variational approach or the density renormalization group approach.

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